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Title: Using Deep Neural Networks to Extract Fireball Parameters from Infrared Spectral Data

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Using Deep Neural Networks to Extract Fireball Parameters from Infrared Spectral Data

ASME 2020 Virtual V&V Symposium
VVS2020-8802

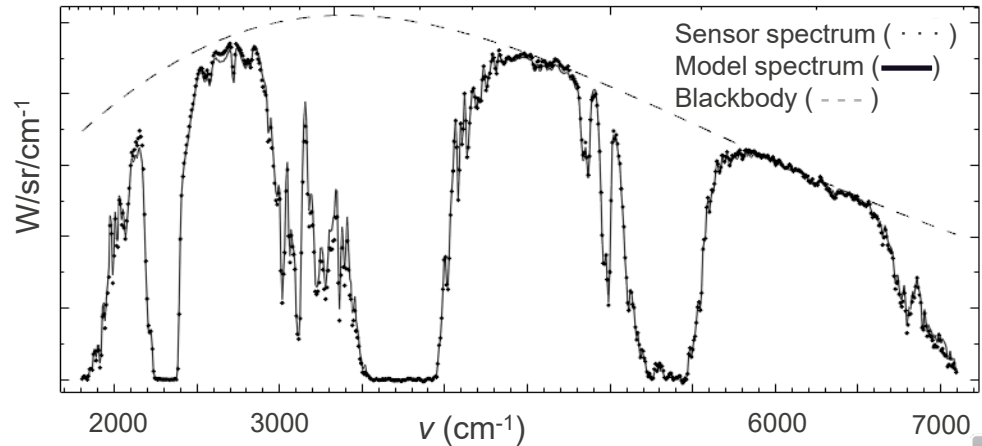
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Joseph G. Gorka, University of Wisconsin – Madison

May 22, 2020



Overview

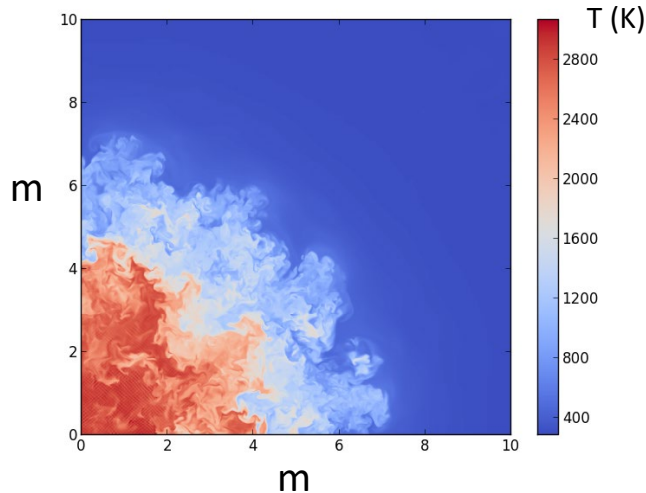
- **Use spectrometers to monitor high explosive (HE) events in infrared region:**
 - Spectrometers measure radiance in many (100s) of spectral bands.
 - Sensors give information on the fireball such as temperature, size, soot quantity and gas species concentrations (CO , CO_2 , H_2O , etc.).



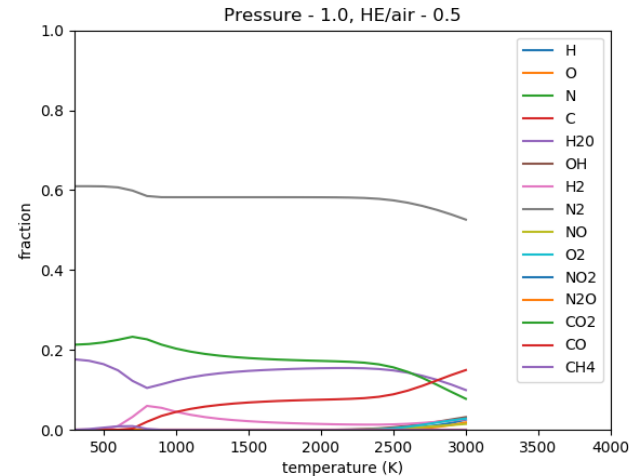
Objective of Data Analysis

- **Develop methods to extract fireball information from remotely sensed infrared data with hundreds of spectral bands.**
 - Recent work looks at machine learning and deep neural networks.
- **Validation of computational physics codes that simulate HE or similar events (equation-of-state (EOS), metal fragmentation, soot).**

Image is 2D slice from 3D simulation

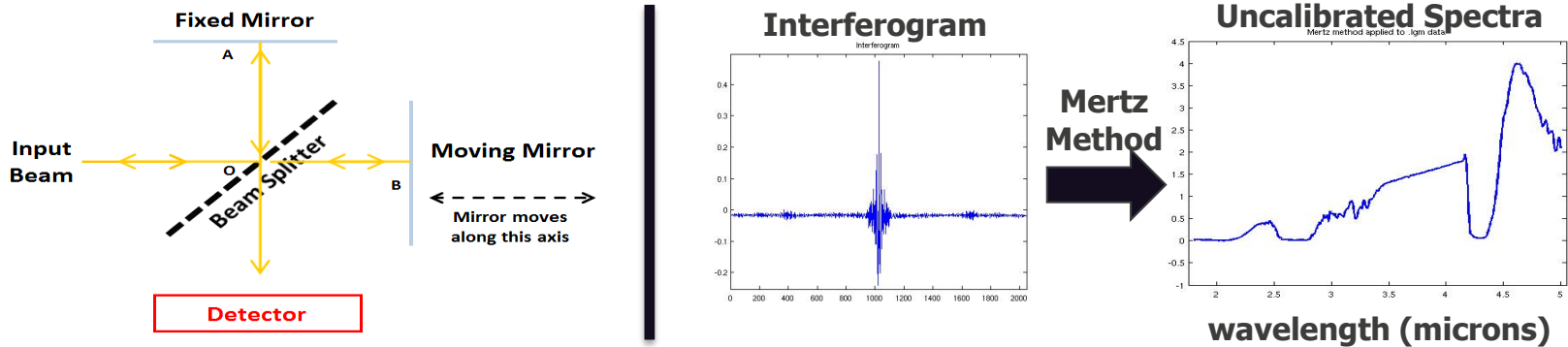


Models for gas species molar fractions in mixed HE/air zones



Spectrometer Resolution and FTIR

- Tradeoff between different resolutions (spatial vs temporal vs spectral):
 - Sensors often sacrifice one type of resolution to improve the other two.
- This presentation considers specific FTIR spectrometer:
 - FTIR (Fourier Transform Infrared): raw data is an interferogram.
 - Single pixel, $\sim 16 \text{ cm}^{-1}$ spectral resolution, $\sim 0.01 \text{ s}$ temporal resolution.



Fireball Radiance Model

At-sensor radiance model $R(\cdot)$ with gas and soot (no additional solid materials):

$$R(\nu) = l^2 \varepsilon_{FB}(\nu) B(T_{FB}, \nu) \tau_{atm}(\nu)$$

$$= \underbrace{l^2}_{\text{area}} \left(1 - \underbrace{e^{-l \kappa_p}}_{\text{soot}} \underbrace{- l \sum \xi_i \sigma_i(\nu)}_{\text{gases}} \right) \underbrace{B(T_{FB}, \nu)}_{\text{Blackbody function}} \underbrace{\tau_{atm}(\nu)}_{\text{Atmospheric transmission}}$$

Fit parameters in red

T_{FB} is fireball temperature

l^2 is fireball area

κ_p is soot absorption coefficient

σ_i is gas cross sections

ξ_i is gas concentrations in $\#/cm^3$

Goal is to find fireball parameters in model $R(\cdot)$ that best fit data.

Methods previously applied: Physics-based fitting, optimization, and Bayesian calibration.



Model for Fireball Radiance

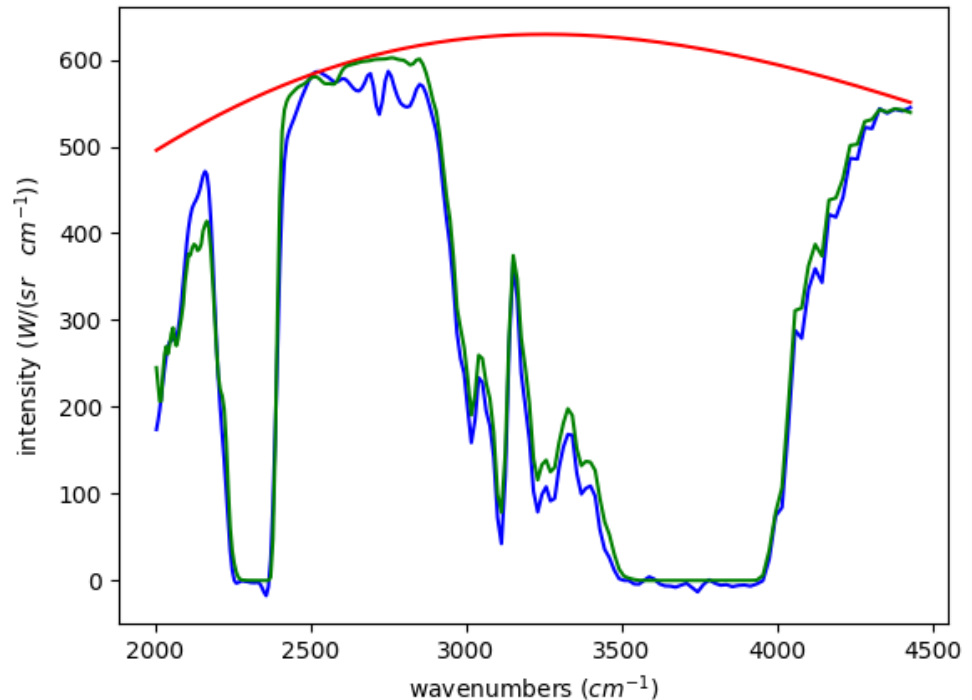
At sensor radiance given by: $R(\nu) = l^2 \varepsilon_{FB}(\nu) B(T_{FB}, \nu) \tau_{atm}(\nu)$

Red curve is blackbody scaled by the fireball area.

Green curve is atmospheric transmission applied to blackbody.

Blue curve is FTIR.

Mismatch between **green** curve and data (**blue**) is due to fireball selective emission from fireball gas constituents.



Computational Challenges

Spectral model is computed at
high resolution: 0.001 cm^{-1}

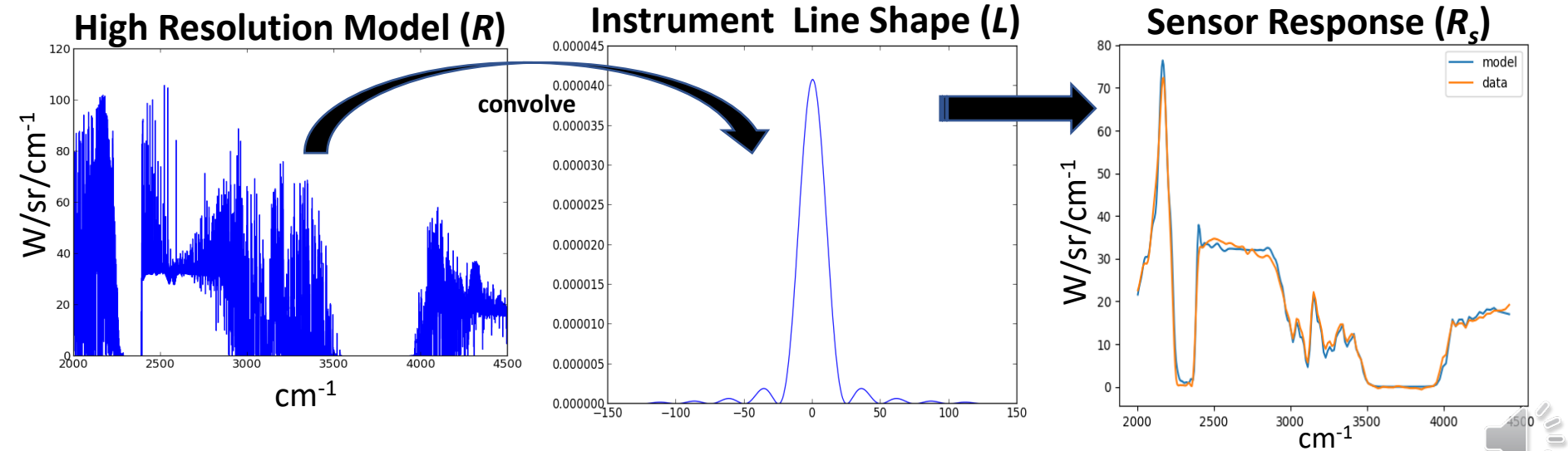
Then convolved with a sensor
response or line-shape L

$T = 1195\text{K}$, $l = 330\text{cm}$,
soot (cm^{-1}) = 0.001,
XH₂O ($\text{\#}/\text{cm}^3$) = $7.3\text{E}17$,
XCO₂ ($\text{\#}/\text{cm}^3$) = $1.7\text{E}18$,
XCO ($\text{\#}/\text{cm}^3$) = $9.2\text{E}16$.

$$R(\nu) = l^2 \varepsilon_{FB}(\nu) B(T_{FB}, \nu) \tau_{atm}(\nu)$$

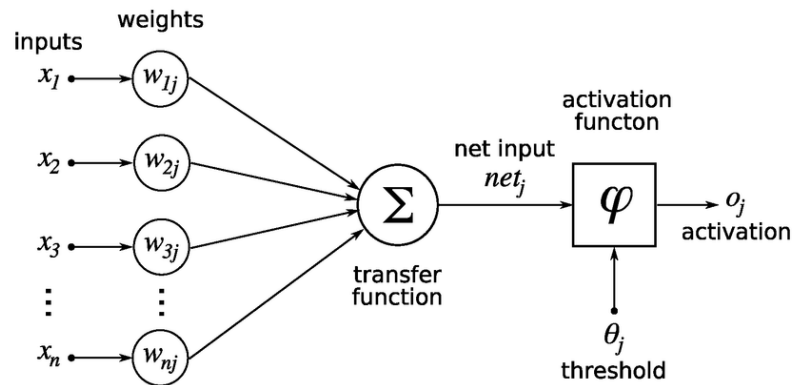
$$R_s(\nu_i) = \int_0^\infty L(\nu - \nu_i) R(\nu) d\nu.$$

$$= l^2 \left(1 - e^{-l \kappa_p - l \sum \xi_i \sigma_i(\nu)} \right) B(T_{FB}, \nu) \tau_{atm}(\nu)$$



Machine Learning

- **Applying machine learning to artificially generated spectra:**
 - Experimental data has no ground truth!
 - Analysis of artificial data to evaluate the accuracy of methods.
- **Deep and shallow learning applied to problem:**
 - Deep learning for full evaluation of regression accuracy.
 - Shallow learning with physics information and determination of important spectral bands.



Generation of Artificial Data Set

- **Data with 388 spectral bands**
~1900 to 5000 cm^{-1}
- **“Easy” data set of ~400,000 artificial spectra:**
 - Diameter kept constant at 3 meters.
 - Additive noise at $\pm 0.5\%$; narrow line-shape.
 - 360,000 for training & testing; 36,000 for validation
- **“Hard” data set of ~400,000 artificial spectra:**
 - All six parameters varied.
 - Additive noise at $\pm 1\%$; wide sensor line-shape.

Parameter	Lower Bound	Upper Bound
T (K)	800	2200
diameter (m)	2	8
soot (cm^{-1})	1E-7	0.04
H ₂ O ($\#/\text{cm}^3$)	1E17	1E18
CO ₂ ($\#/\text{cm}^3$)	1E17	2E18
CO ($\#/\text{cm}^3$)	1E14	1E17

Data generated by sampling each parameter uniformly, except for soot.

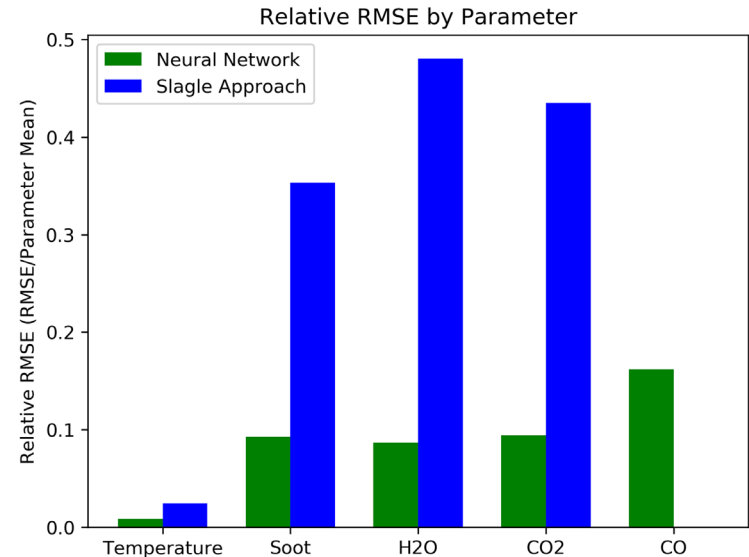
Soot sampled such that the emissivity due to soot is uniform.



Deep Learning on Artificial Data

Tested NN with many layers, including convolutional layers.

Construction of Neural Network		
Layer	Output Shape	Parameter Count
1D Convolution (Input)	(193, 16)	64
1D Convolution	(96, 32)	1568
1D Convolution	(47, 64)	6208
1D Convolution	(23, 128)	24704
1D Convolution	(23, 16)	2064
Flatten	(None, 368)	0
Dense	(None, 500)	184500
Dense	(None, 250)	125250
Dense	(None, 50)	12550
Dense (Output)	(None, 5)	255



Compared results to Physics-based method of Slagle (AFIT thesis, 2009).

Fireball area kept constant to make problem easier (T, area, and soot are highly correlated)

Networks with Single Hidden Layer

- **What would the results be with a single hidden layer (HL)?**
 - How many nodes/neurons are necessary for a good model?
 - Convolutional layers are counter-intuitive, especially for uncovering gases.

Fireball area kept constant.

S1 is RMSE/mean.

S2 is average relative error.

Validation statistics obtained from a set of 36000 artificial spectra.

Number of neurons for single HL varied from 128 to 2048 in a grid search.

Parameter	Deep NN S1	Single HL S1 / S2
T	0.009	0.009 / 0.008
soot	0.093	0.070 / 0.091
H2O	0.087	0.114 / 0.097
CO2	0.094	0.110 / 0.111
CO	0.160	0.165 / 0.420



Results with Varying Fireball Size

- **Temperature, fireball diameter, and soot quantity are highly correlated:**
 - All three impact magnitude of fireball radiance.
 - Soot is a gray-body (emission is independent of wavenumber).
 - Hard to include all three as unknown in the data.

Data 1: fireball size kept constant.

Data 2: all parameters vary.

Validation statistics obtained from a set of 36000 artificial spectra.

For soot and gases, output labels y transformed by $\log(y)$.

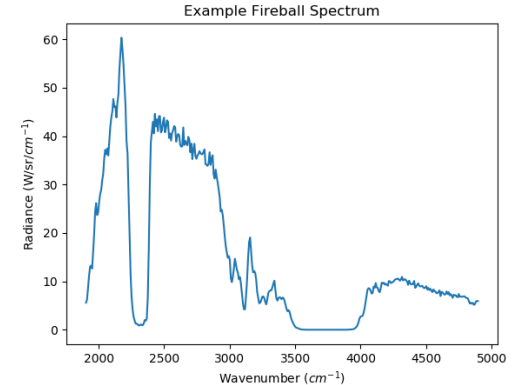
Parameter	“Easy” Data 1 S1 / S2	“Hard” Data 2 S1 / S2
T	0.009 / 0.008	0.006 / 0.004
diameter	NA	0.012 / 0.009
soot	0.070 / 0.091	0.240 / 0.050
H ₂ O	0.114 / 0.097	0.203 / 0.141
CO ₂	0.110 / 0.111	0.286 / 0.199
CO	0.165 / 0.420	0.522 / 0.656



Are Better Results Possible?

- **Why do the gases become harder to estimate?**

- Radiance is a smooth function of temperature, size, and soot.
- Would think that estimators could discern gases from non-smooth structure across bands.



- **Tested compensating data for temperature and size:**

- Build estimator for T and size.
- Apply to a data set, divide out impact of T and size, then fit to the other parameters.

$$\frac{R(\nu)}{l^2 B(T_{FB}, \nu)} = \varepsilon_{FB}(\nu) \tau_{atm}(\nu)$$

THIS DID NOT WORK! RESULTS WERE WORSE!

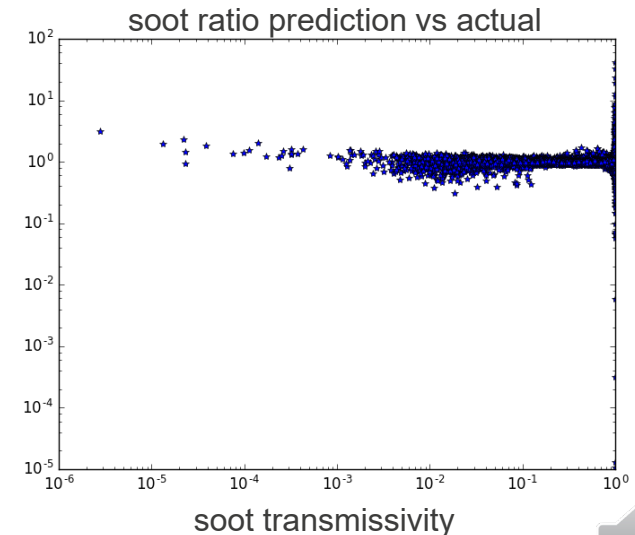
Are the Results Misleading?

If soot concentration is large enough, estimates for the gases are unreliable:

- Soot makes the fireball opaque: $R(v) = l^2(1 - e^{-l\kappa_p - l \sum \xi_i \sigma_i(v)})B(T_{FB}, v)\tau_{atm}(v)$
- Should estimate emissivity of soot and if it's close to one, then it is likely that the gas estimates have high uncertainty.

Create a new label (output) equal to soot transmissivity $e^{-l\kappa_p}$:

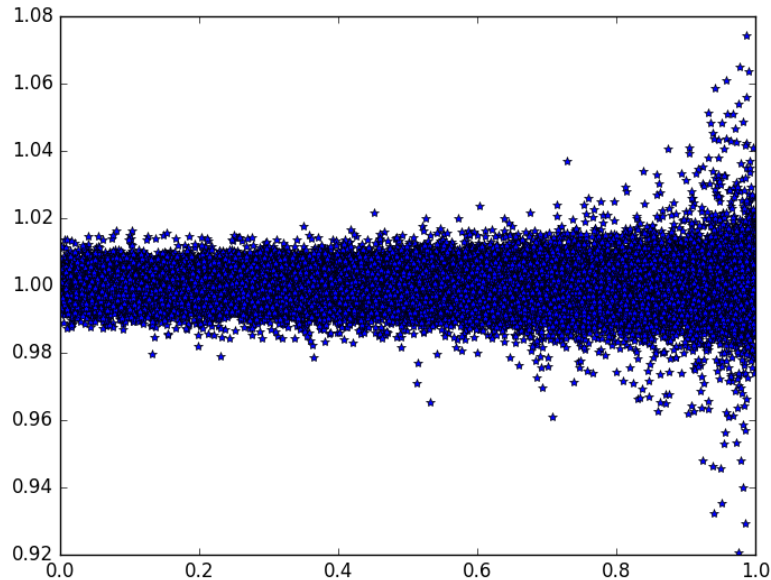
Training single HL network on this output resulted in RMSE of **0.039** on a validation set.



Soot's Impact on T and Size

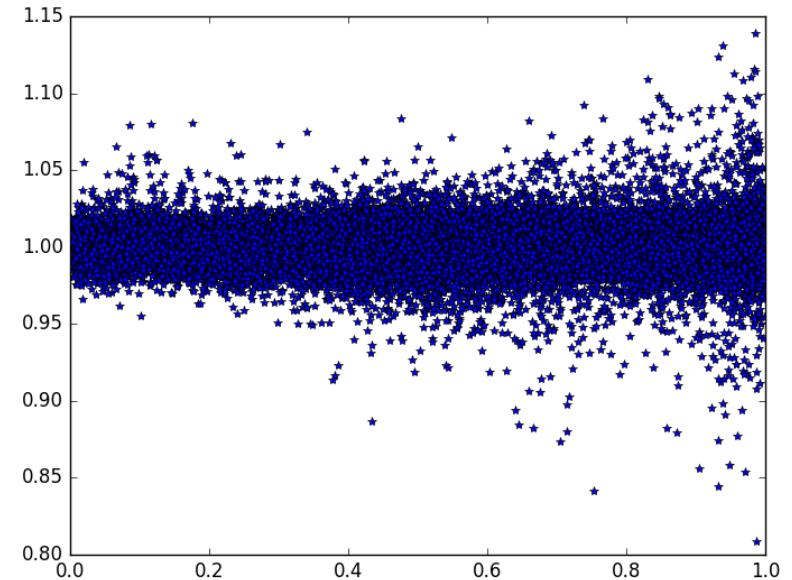
Results from a validation data set.

T ratio prediction vs actual



soot transmissivity

diameter ratio prediction vs actual

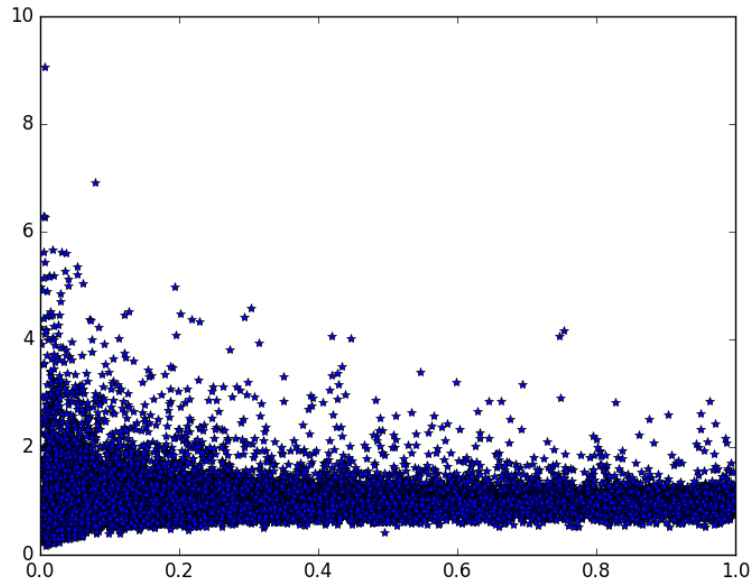


soot transmissivity



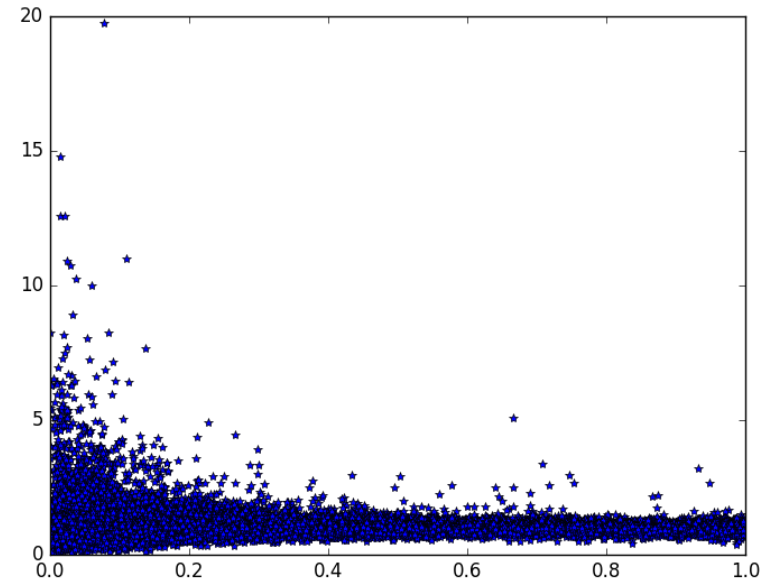
Soot's Impact on H₂O & CO₂

H₂O ratio prediction vs actual



soot transmissivity

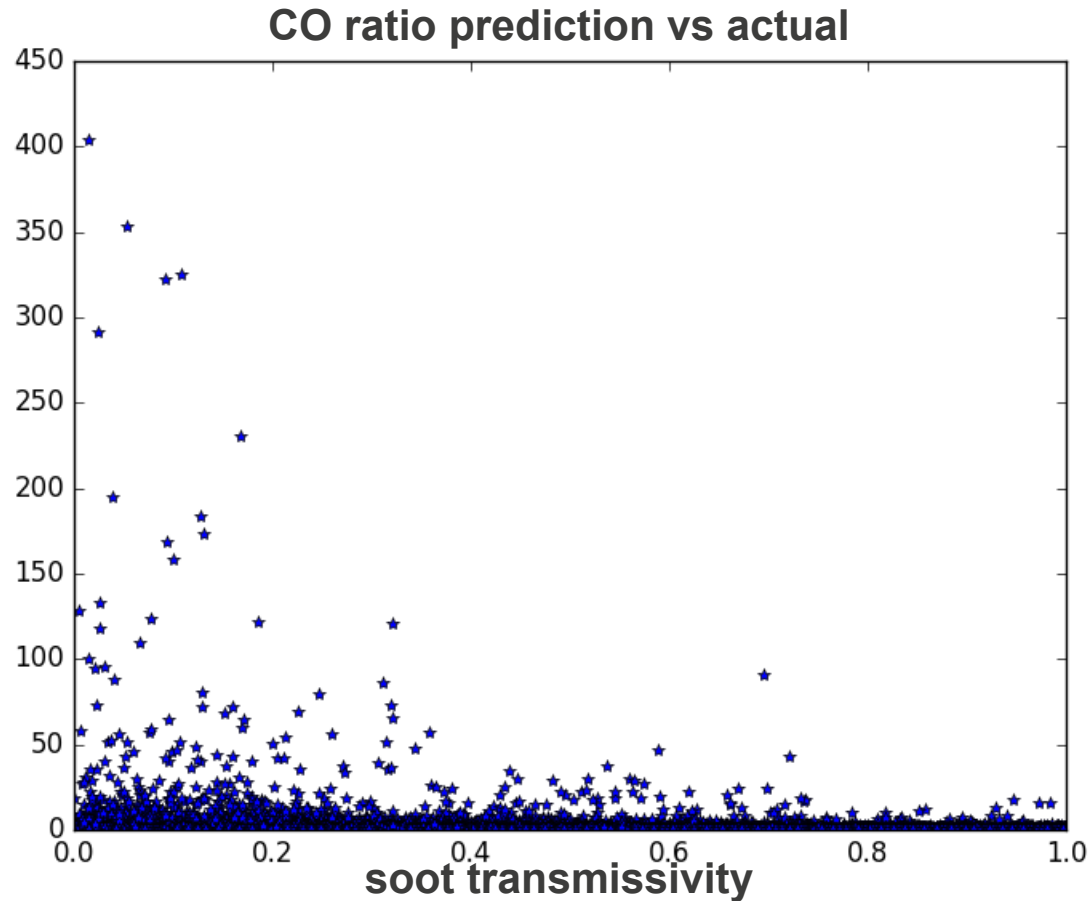
CO₂ ratio prediction vs actual



soot transmissivity



Soot's Impact on CO



Conclusion

- **Next Step (1): Examine outliers in prediction.**
 - Why is it difficult to predict the fireball parameters for some spectra?
- **Next Step (2): Reverse fitting to uncover most “important bands”**
 - Train a network to predict spectral band given the six parameters.
 - Bands that can be accurately predicted are “important”.
- **Analyzing artificial fireball spectra:**
 - Develop methods for recovering fireball parameters.
 - Validation and improvement of computational physics codes.

